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FILE

#### MEMORANDUM FOR PRS (Contractor Publication)

FROM: PROI (STINFO)

19 May 2003

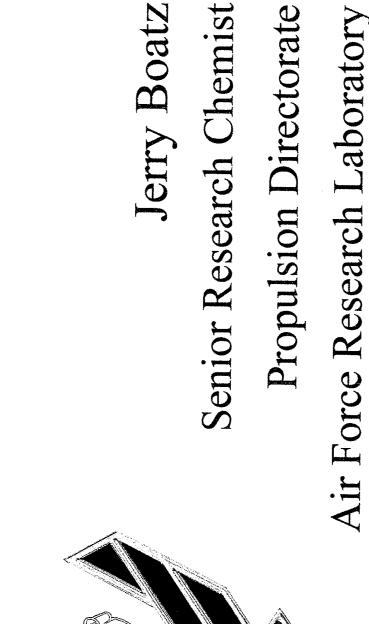
SUBJECT: Authorization for Release of Technical Information, Control Number: AFRL-PR-ED-VG-2003-138

Boatz, Jerry (PRSP), "New Materials Design"

DoD High Performance Computing Users Group Conference (Bellevue, WA, 9-13 Jun 2003) (Deadline = 9 Jun 2003)

(Statement A)

#### New Materials Design DoD UGC, 9-13 June 2003 Bellevue, WA





### NEW MATERIALS DESIGN



#### THE TEAM...

Prof. Mark S. Gordon

Prof. Gregory Voth



Prof. Sharon Hammes-Schiffer



Dr. Ruth Pachter, AFRL/MLPJ



Dr. Jerry Boatz, AFRL/PRSP





#### OUTLINE

#### 1. Project Overview

- High energy density materials
- Polyhedral oligomeric silsesquioxanes (POSS)
- Non-linear optical materials

### 2. Theoretical Methods and benchmarks

- Ab initio electronic structure theory
- Nuclear-electronic orbital approach

#### 3. Results

#### 4. Summary

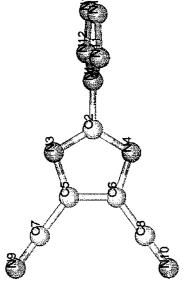


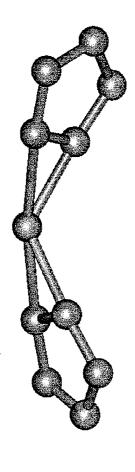


## PROJECT OVERVIEW - HEDM

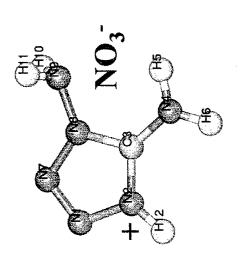


# High Energy Density Matter -- next generation rocket propellants





High-nitrogen/polynitrogen compounds



Energetic Ionic Liquids



4



## PROJECT OVERVIEW - HEDM



## Technical issues being addressed using CCM

### 1. High-nitrogen/polynitrogen compounds

Objective: identify, characterize, and synthesize stable compounds with high heats of formation, high densities

- geometries, energy content, stabilities, reaction pathways

#### 2. Energetic ionic liquids

Objective: identify, characterize, and synthesize thermally stable energetic ILS with low melting points, high densities and low viscosities.

geometries, electronic structures, stabilities, energy content, interaction potentials

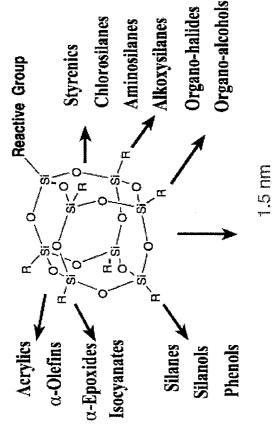


## PROJECT OVERVIEW - POSS



# Polyhedral oligomeric silsesquioxanes -- next generation plastics

#### Molecular Silica



#### As Additives

Mechanical property/viscosity/thermal modifiers Heat/abrasion resistant paints and coatings

Crosslinking agents

#### Fire retardants

As Plastics

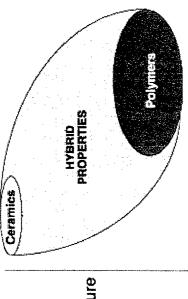
Space resistant resins Electronic materials Packaging/coatings Medical materials

Optical Plastics

#### As Preceramics

Ablative materials (nozzles, insulations etc.) Precursors to glassy or ceramic matrices Claddings/electronics coatings

#### HYBRID POLYMERS



**Toughness** 

S nm

Temperature

ဖ



## PROJECT OVERVIEW - POSS



## Technical issues being addressed using CCM

#### 1. Mechanisms of formation

Objective: rational design and synthesis of POSS

- role of solvents, acid/base catalysis, substituent effects on mechanism of formation

### 2. Potential applications as molecular "sieves"

Objective: determine if POSS cages can be used to separate small molecules

- determine barriers to encapsulation of  $N_2$  and  $O_2$ 

#### 3. Ti-POSS as new catalysts

Objective: determine if Ti-POSS and Ti-siloxane compounds are effective catalysts

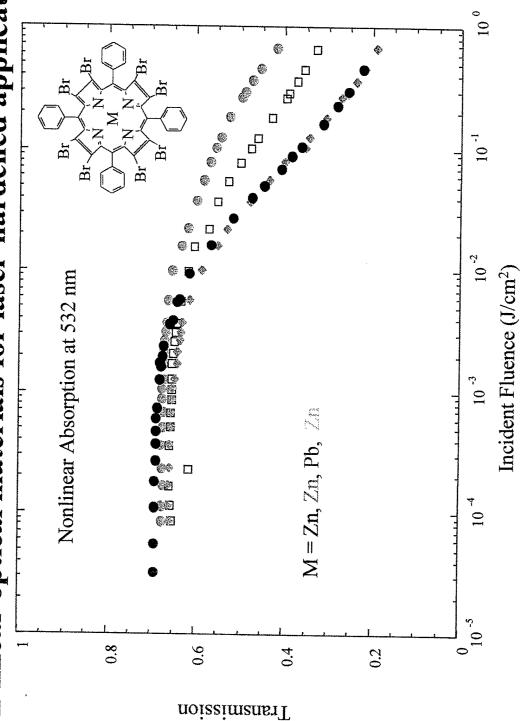
determine barriers to polymerization of ethylene, oxidation by HOOH.



### PROJECT OVERVIEW - NLO







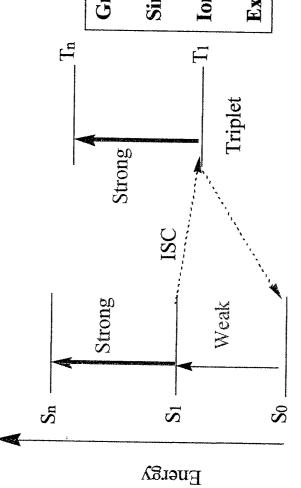


### PROJECT OVERVIEW - NLO



## Technical issues being addressed using CCM

## 1. Mechanism of reverse saturable absorption (RSA)



### Key Components of RSA

Ground state spectra (linear response)

Singlet-triplet splittings (ISC, phosphorescence)

Ionization potential (photoionization)

Excited triplet spectra (NLA)

Singlet

Five-level model for nonlinear absorption





### 1. Ab initio electronic structure theory

- General Atomic and Molecular Electronic Structure System (GAMESS) -- a CHSSI code
- Nuclear-electronic orbital approach (NEO) for including nuclear quantum effects (important, e.g., in proton transfer reactions)

molecular electronic Schrödinger equation from quantum mechanics: Various computational techniques are employed to solve the

$$-\frac{1}{2}\sum_{i}\nabla_{i}^{2} - \sum_{i}\frac{Z_{\alpha}}{\alpha} + \sum_{i}\sum_{j>i}\frac{1}{r_{ij}}\left|\Psi_{el} = E_{el}\Psi_{el}\right|$$

Categories of approximate solutions:

- a) "Self-consistent field" (SCF): reasonably good geometries
- b) "Electron correlation": post-SCF correction, required for reliable energetics (e.g., barriers).







1. Ab initio electronic structure theory (cont.)

"clampled nuclei") approximation -- NOE method treats specified - Most electronic structure codes use Born-Oppenheimer (i.e., nuclei at QM level.

### Nuclear-Electronic Hamiltonian

$$H_{\text{tot}}(\mathbf{r}_{e}, \mathbf{r}_{q}; \mathbf{r}_{c}) = -\sum_{i}^{N_{e}} \frac{1}{2} \nabla_{i}^{2} - \sum_{i}^{N_{e}} \sum_{A}^{N_{c}} \frac{Z_{A}}{r_{iA}} + \sum_{i}^{N_{e}} \sum_{J>i}^{N_{e}} \frac{1}{r_{iJ}}$$
$$-\sum_{I}^{N_{p}} \frac{1}{2M_{I}} \nabla_{I}^{2} + \sum_{I}^{N_{p}} \sum_{A}^{N_{c}} \frac{Z_{A}Z_{I}}{r_{IA}} + \sum_{I}^{N_{p}} \sum_{J>I}^{N_{p}} \frac{Z_{I}Z_{J}}{r_{IJ}}$$
$$-\sum_{i}^{N_{e}} \sum_{I}^{N_{p}} \frac{Z_{I}}{r_{iI}} + \sum_{A}^{N_{c}} \sum_{A>A}^{N_{c}} \frac{Z_{A}Z_{B}}{r_{AB}}$$

 $N_e$ : number of electrons (coordinates  ${f r}_e)$ 

number of quantum nuclei (coordinates  $\mathbf{r}_p)$ 

number of classical nuclei (coordinates  $\mathbf{r}_c)$ 







#### Current Status of parallel GAMESS Ab initio electronic structure theory

	用	ROHF	뷤	GVB	MCSCF
Energy	dpo	cdp	dpo	dpo	dpo
Analytic Gradient	dpo	dpo	cdp	dpo	cdp
Numeric Hessian	cdp	dpo	cdp	dpo	cqb
Analytic Hessian	cdp	cdp	ı	cdp	•
MP2 energy	cdp	dpo	dpo	I	d o
MP2 gradient	cdp	1	po	ı	ı
Cl energy	cdp	dpo	1	dpo	dpo
Cl gradient	cq	ŧ	ı	ī	ı
DFT energy	cqb	dpo	cdp	ī	
DFT gradient	cdp	dpo	cdp	ı	ŧ

c = conventional disk storage of AO integrals

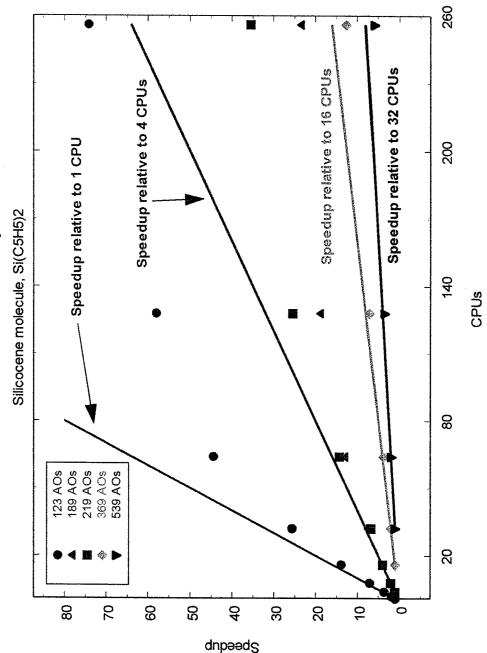
d = direct evaluation of AO integrals

p = runs in parallel



#### MP2 Gradient Scalability Test

Ab initio electronic structure theory







## The Search for New Polynitrogens



- All polynitrogens are unstable with respect to N<sub>2</sub> molecules
- Their activation energy for N<sub>2</sub> elimination is largely determined by the weakest bond in the compound
- Their metastability is enhanced if suitable resonance structures exist:

$$[N-N=N] \longleftrightarrow [N=N-N] \longleftrightarrow [N-N-N]$$

- The double-bond character of the N—N bonds in the azide anion explains its exceptional stability
- How can this stabilization effect be used to our advantage in preparing new compounds?



### Pentazolate (N<sub>5</sub>-)?

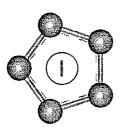


- Substituted pentazoles R-N<sub>5</sub> have been known for decades (R=aryl)
- Cyclic N<sub>5</sub> is aromatic
- Conversion of the diazonium salt,  $RN_2^+$ , to the substituted pentazole ring R- $N_5$  by the reaction with azide ion, N<sub>3</sub>-, has been demonstrated many years ago by Ugi and Huisgen.
- N<sub>5</sub>- has been recently detected in the gas phase for the first time, using collisional fragmentation (electrospray ion mass spectroscopy).
- Can a chemical route to N<sub>5</sub>- be found? (e.g., can a suitable R group be found for the reaction  $R-N_2^+ + N_3^- -> R-N_5^- -> R^+ + N_5^-$ ?



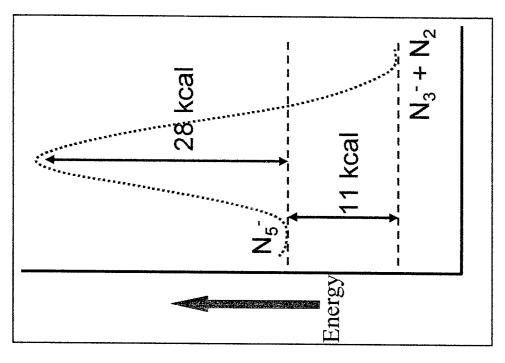
### New Polynitrogen Anions





#### Pentazole anion (N<sub>5</sub>-)

- Theoretical calculations show that this anion has a 28 kcal/mole activation energy barrier for decomposition and its decomposition to N<sub>3</sub><sup>-</sup> and N<sub>2</sub> is only 11 kcal/mol exothermic
- Aryl substituted pentazoles can be isolated temperature to form aryl azides and N<sub>2</sub> gas as stable compounds only if stored at low compounds rapidly decompose at room temperatures. In methanol, these



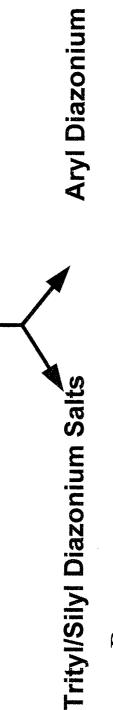


### Synthetic Challenge – How do we make These New Anions??

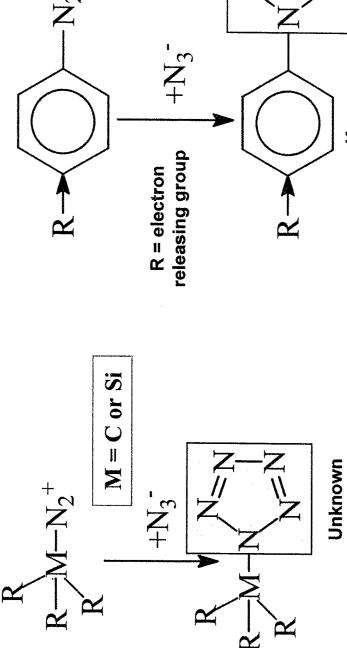


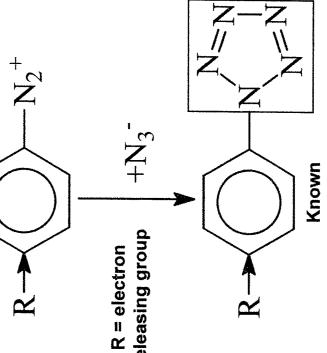
## Synthesis of Substituted Pentazoles

Sources for the Pentazole Anion (N<sub>5</sub>-)



**Aryl Diazonium Salts** 







### Theoretical Challenge - Can we design and predict viable precursors to $N_5$ ?



Find a substituent R so that

- 1. R-N<sub>2</sub><sup>+</sup> is stable wrt R<sup>+</sup> + N<sub>2</sub>.
- 2. The R-N bond in R-N<sub>5</sub> is weak, thereby suitable for the reaction R-N<sub>5</sub> + M<sup>+</sup>X<sup>-</sup> -> M<sup>+</sup>N<sub>5</sub> + R-X

#### Approach

stability of R-N<sub>2</sub><sup>+</sup> diazonium salts and the length/strength Use quantum chemical calculations to predict the of the R-N<sub>5</sub> bond.

MBPT(2)/6-31G(d) level of theory

$$L_3M-N_2^+$$

$$M = C, Si$$

$$L = F$$
, CI, CH<sub>3</sub>, CF<sub>3</sub>, NO<sub>2</sub>, phenyl, etc.



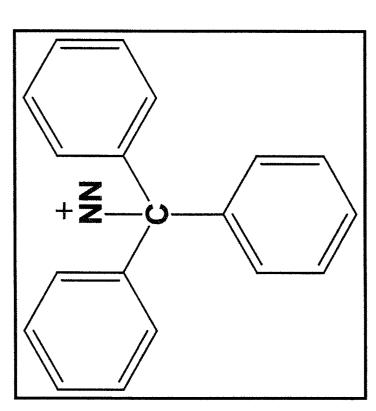


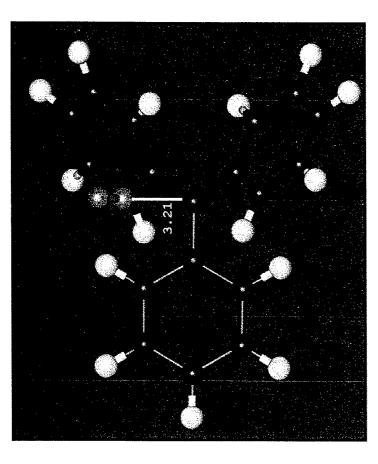
## Identifying Precursors for New Polynitrogens



This ion has been suggested as a useful precursor to new polynitrogen molecules...

» ... but calculations predict it to be unstable.





Computational requirements: ~50,000 CPU-hours, 1.2 GW on IBM SP/P3 at ASC



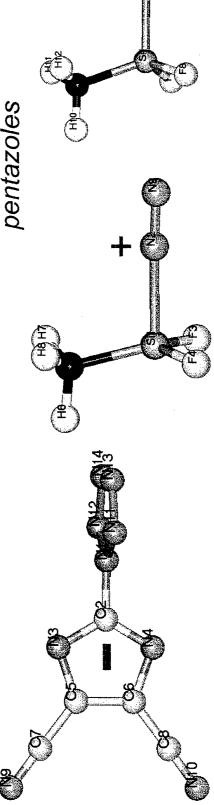
### RESULTS - HEDM

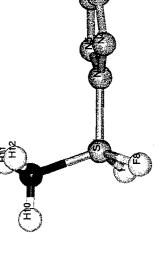


### High-nitrogen/polynitrogen compounds

precursor to displacement of N<sub>5</sub>-Potential dicyanoimidazolate

Potential diazonium  $[R_3Si-N_2]^+$  precursors to formation of suitable  $R_3Si-N_5$  substituted





ھے	R <sub>3</sub> Si-N <sub>2</sub> <sup>+</sup> distance(Å)	D <sub>e</sub> (Si- N <sub>2</sub> +) (kcal/mol)	R <sub>3</sub> Si-N <sub>5</sub> distance (Å)
3Ме	2.151	13.8	1.855
2Me,F	2.144	15.7	1.834
Me,2F	2.151	21.2	1.855
3F	1.973	33.4	1.783

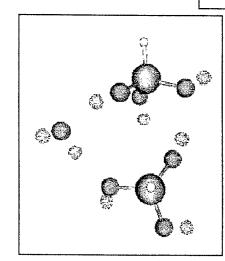
Computational requirements: ~50,000 CPU-hours, 1 GW on IBM SP/P3 at ASC



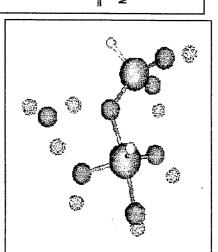


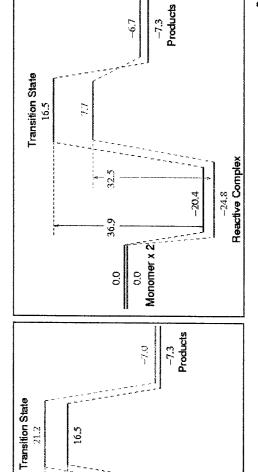
# Nuclear quantum effects in water-catalyzed condensation reactions

$$2 \times HSi(OH)_3 + H_2O \rightarrow H(OH)_2Si-O-Si(OH)_2H + 2H_2O$$



	Keactive	Iransition		$C_{r}^{r}$
Level	Complex	State	Products	Time
RHF/6-31G*		16.5	-7.3	1.0
RHF/6-31G*/ZPE	9.6	C. C	-7.0	
NEO/HF/4		7.2	-5.9	1.1
NEO/HF/8	-24.8	7.7	<b>L.9</b> —	1.8





Reactive Compley



### POSS as catalysts?

Some Ti compounds are know to be effective catalyts Ziegler-Natta, olefin oxidation Recent experiments reveal Ti-modified silicates catalyze olefin oxidation by peroxides Can Ti-substituted siloxanes and/or POSS catalyze olefin oxidation by HOOH, or polymerization?







### POSS computational methods



§ Hessians to characterize stationary points

§ Energies using MP2/TZVP

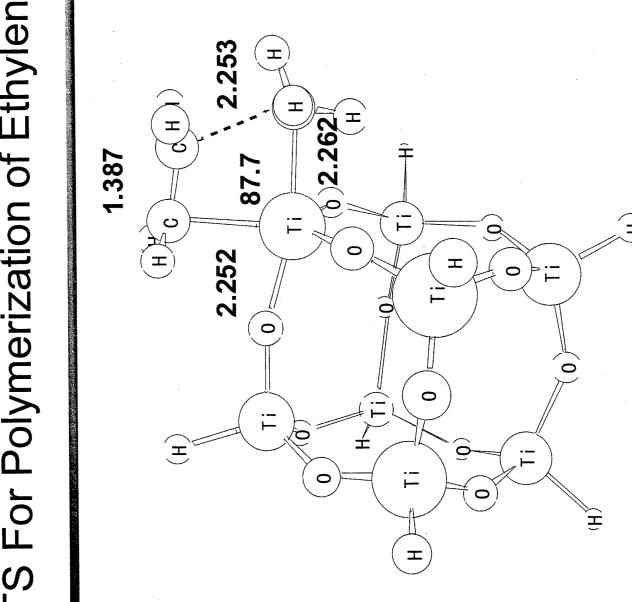
§ Some geometries re-optimized with MP2

§ Size of basis set: ~1,000 basis functions

§ Calculations performed at ERDC (T3E) and AHPCRC (T3E)

## TS For Polymerization of Ethylene





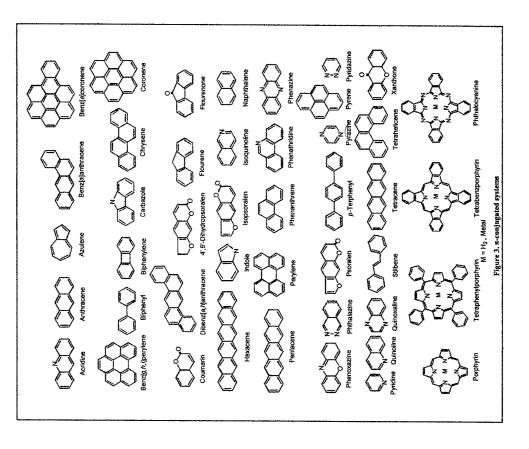




#### RESULTS - NLO



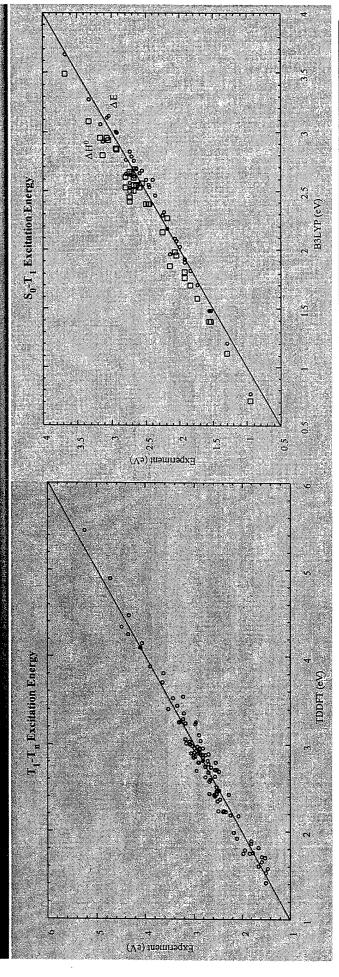
Systematic investigation of excited state energies and oscillator strengths of free-base porphyrins, phthalocyanines, and their metal complexes, representing a broad range of  $\pi$ -conjugated systems, using time-dependent density functional theory (TD-DFT).





#### RESULTS - NLO





Computed T<sub>1</sub>-T<sub>n</sub> compared to experimental results

86 Experimental Values (in solution) Mean Absolute Error = 0.11 Maximum Error = 0.31

Computed S<sub>0</sub>-T<sub>1</sub> compared to experimental results

47 Experimental Values (in solution)
Mean Absolute Error = 0.14
Maximum Error = 0.33



#### SUMMARY



### High Energy Density Matter

- High-nitrogen/polynitrogen compounds are substantially more energetic than hydrazine.
- Trityldiazonium cation is not a stable polynitrogen precursor.
- Trimethylsilyldiazonium cation is marginally stable, replacement of methyls with fluorines increases stability.

## Polyhedral Oligomeric Silsesquioxanes (POSS)

- Nuclear quantum effects are important in proton transfer reactions -- lower barriers by about 4 kcal/mol for water-assisted condensation of trisilanol
- Most effective catalyst for olefin polymerization is T<sub>4</sub> cage
- Barrier is still ~10 kcal/mol too high: Ti-POSS, Ti-siloxanes may not be good catalysts for this reaction

#### **NLO** materials

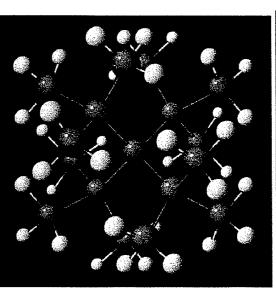
- Time-dependent density functional theory accurately predicts NLA in free-base porphyrins, phthalocyanines, and their metal complexes.
- Mean absolute error of 0.11 eV for computed triplet-triplet excitation energies
- Mean absolute error of 0.14 eV for computed singlet-triplet excitation energies

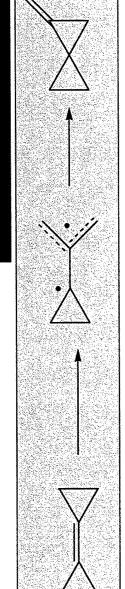
### FUTURE DIRECTIONS



#### HEDM

- Thermal decomposition mechanisms of energetic hydrocarbons (e.g., BCP).
- Energetic Ionic Liquids (QSPR models)









### ACKNOWLEDGEMENTS



POSS: Takako Kudo, Shawn Phillips, Simon Webb, Frank Feher, Joe Lichtenhan

HEDM: Jeff Mills, Greg Drake, Karl Christe, Bill Wilson, Ashwani Vij, Vandana Vij

NLO: Kiet Nguyen, Paul Day

GAMESS: Graham Fletcher

MSRCs, DCs: ASC, ARL, ERDC, NAVO, MHPCC, AHPCRC, ARSC, AFFTC

CHSSI funding (CCM-2, CCM-4, MBD-01)



#### **Backup Slides**



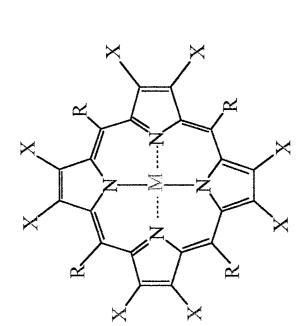


## PROJECT OVERVIEW - NLO



## Technical issues being addressed using CCM

2. "Tuning" of absorption spectrum by benzannulation, halide substitution



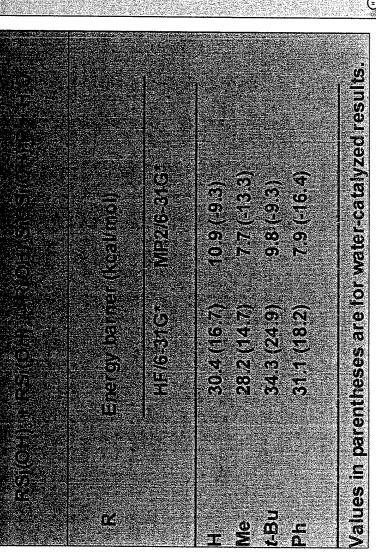
System					Proj	Property	
		×	~	IIP	$S_{0}$ - $S_{n}$	$S_0$ -T1	$T_{1}$ - $T_{1}$
PH2	四の日	H	H	E, C	E, C	E, C	E, C
ZnP	N. III	H	H	E, C	E, C	E, C	E, C
TPPH2	Zm	H	<b>→</b>	E, C	E, C	E, C	E, C
ZnTPP	Z		<b>-</b>	E, C	E, C	E, C	E, C
ZnTPPBr8	No.	Br.	-	C	E, C	E, C	E, C

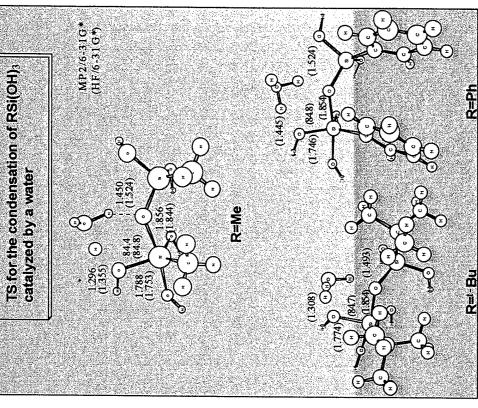
IP = Ionization Potential,  $S_0$ - $S_n$  = Ground State Spectrum,  $S_0$ - $T_1$  = Singlet-Triplet Gap  $T_1$ - $T_n$  = Triplet-Triplet Spectrum E = Experiment, C = Calculated





# Mechanism of formation: role of solvent (H<sub>2</sub>O) & substituents (R





Kudo, T., Gordon, M.S. J. Am. Chem. Soc., 120, 11432 (1998) Kudo, T., Gordon, M.S. J. Phys. Chem. A, 104, 4058 (2000)





### Mechanism of formation

#### Key steps

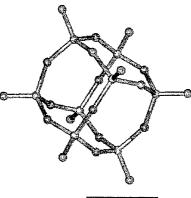
1. Hydrolysis of RSiX<sub>3</sub> (R=H,CH<sub>3</sub>,t-butyl,etc.; X=Cl)  $RSiCl_2OH + H_2O \rightarrow RSiCl(OH)_2 + HCl$  $RSiCl_3 + H_2O \rightarrow RSiCl_2OH + HCI$ RSiCl(OH)<sub>2</sub> + H<sub>2</sub>O  $\rightarrow$  RSi(OH)<sub>3</sub>

 $2 \text{ RSi(OH)}_3 \rightarrow \text{R(OH)}_2 \text{SiOSi(OH)}_2 \text{R} + \text{H}_2 \text{O}$ 2. Condensation of  $RSi(OH)_3$  to disiloxane

 $RSi(OH)_3 + R(OH)_2SiOSi(OH)_2R \rightarrow D_3 + 2H_2O$ 3. Condensation of disiloxane to  $D_3$ , $D_4$ 

[3+1]: RSi(OH)<sub>3</sub> + R(OH)<sub>2</sub>SiOSi(OH)<sub>2</sub>R  $\rightarrow$  D<sub>4</sub> + 2H<sub>2</sub>O Ring Expansion:  $RSi(OH)_3 + D_3 \rightarrow D_4 + H_2O$ [2+2]:  $2R(OH)_2SiOSi(OH)_2R \rightarrow D_4 + 2H_2O$ 

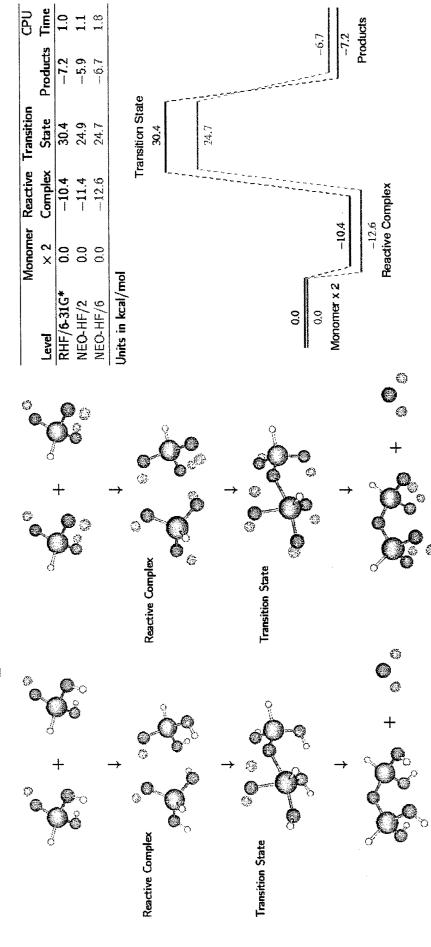
4. Condensation of  $D_3$ ,  $D_4$  to POSS (in progress)







## Nuclear quantum effects in condensation reactions

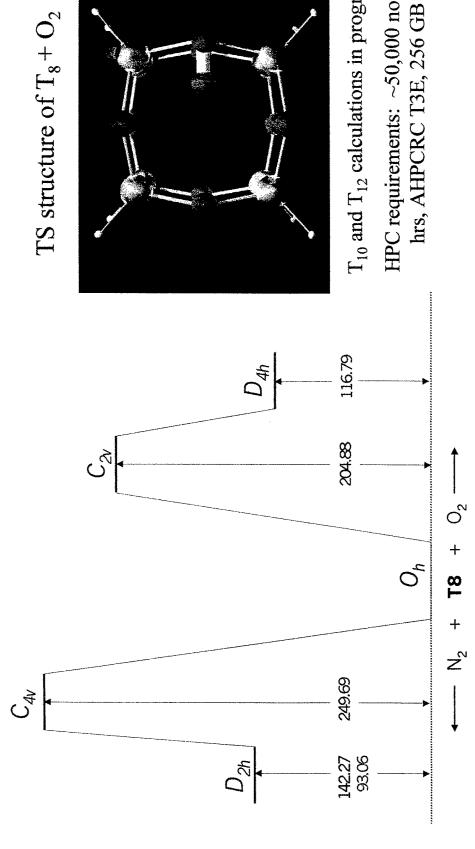


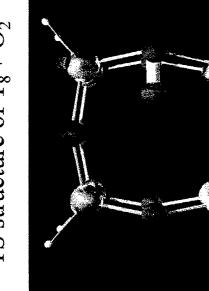
Webb, S.P., Agarwal, P.K., and Hammes-Schiffer, S. J. Phys. Chem. B, 104(2000), 888 Webb, S.P. and Hammes-Schiffer, S. 1 Chem. Phys. 113 (2000), 5214 Hammes-Schiffer, S. J Phys Chem. A 102 (1998), 10443





## Molecular "sieves": preferential capture N2 vs. O2?





 $T_{10}$  and  $T_{12}$  calculations in progress HPC requirements: ~50,000 node-





#### RESULTS - NLO

### B3LYP S<sub>0</sub>-T<sub>1</sub> Excitation Energies (in eV)

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System	6-31G(d)	Error	Exp
Porphyrin (1 <sup>3</sup> B <sub>2u</sub> )	1.42	0.16	1.58a
Zinc Porphyrin (1 <sup>3</sup> B <sub>1u</sub> )	1.65	0.07	1.72b
Tetraphenylporphyrin (1 <sup>3</sup> B <sub>1</sub> )	1.31	0.14	1.45 <sup>c</sup>
Zinc Tetraphenylporphyrin(13B1)	1.53	90.0	1.59d
Zinc Phthalocyanine (1 <sup>3</sup> B <sub>2u</sub> )	1.05	80.0	1.13e
Zinc Tetrabenzporphyrin (13B1u)	1.41	0.16	1.57f
Phthalocyanine (1 <sup>3</sup> B <sub>1u</sub> )	1.18	90.0	1.248
Mean Error		0.10	

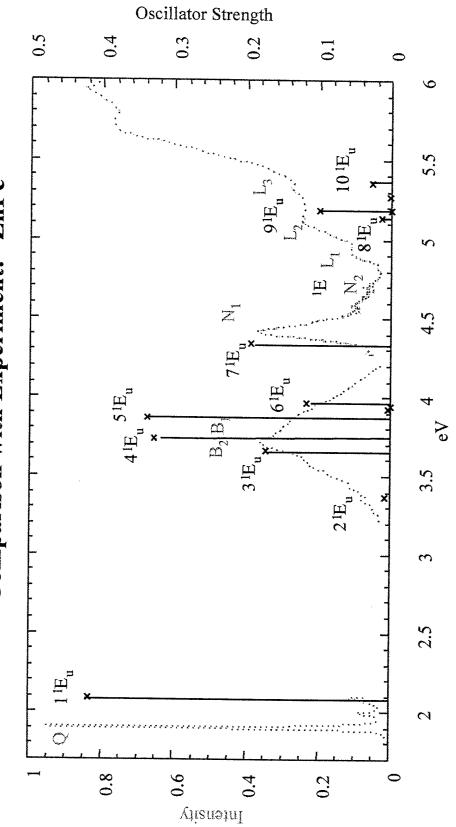
Gouterman, J. Mol. Spectrosc. 1971, 39, 421 (octane at 77 K) EMcVie et al., J. Chem. Soc. Faraday Trans. II 1978, 74, "Gouterman, Khalil, J. Mol. Spectrosc. 1974, 53, 88. (EPA (5:5:2) mixture of ethyl ether to isopentane to ethanol) ether to ethanol at 77 K) "Vincett et al., K. E. J. Chem. Phys. 1971, 55, 4131. (1-chloronapthalene at 77 K) Bajema, Khalil, J. Mol. Spectrosc. 1974, 53, 88. (EPA at 77 K) dWalters et al., J. Phys. Chem. 1995, 99, 1166.(1:1 mixture of and 50% ethyl iodide at 77 K) bGradyushko, Tsvirko, Opt. Spectrosc. 1971, 31, 291. (EPA at 77 K) 'Gouterman, 1870 (1-chloronapthalene at 77 K)

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#### RESULTS - NLO







HPC Requirements: ~100,000 CPU hours, on SGI O2K + IBM SP3 + SGI O2K @ ASC

